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Discrete Optimization of a Styrene Production Process

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DISCRETE OPTIMIZATION OF A STYRENE PRODUCTION PROCESS

by
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A thesis submitted to the faculty of The University of Mississippi in partial fulfillment of the requirements of the Sally McDonnell Barksdale Honors College.

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ABSTRACT

This thesis will outline the two phases of my capstone design project for Chemical Engineering. The first goal was to simulate a styrene production process in Excel alongside my group members in ChE 451. During this phase, we looked at startup of the process and the first 12 years of operation. After the base case which included an isothermal reactor, the decision was made to switch to an adiabatic reactor based on net present value evaluations. Discrete optimization took place on the adiabatic reactor and the subsequent process. The second phase of my capstone project was the portion assigned to fulfill the requirements of the Sally McDonnell Barksdale Honors College Senior Thesis. To complete these requirements, my thesis group was tasked with simulating a fluidized bed reactor. After completion of the calculations for the reactor we were able to do an economic analysis. To compare the fluidized bed reactor and the isothermal/adiabatic reactors, we calculated the estimated annual operating costs. The specific details of this process is the subject of discussion within my thesis.

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I. Summary of Chemical Engineering Design and Optimization

When designing a chemical process the two most important steps are process design and process optimization. There are generally seven steps in the setup of a new process design. First, one must identify the objective and set the design basis. The next step is to generate possible design concepts. These projects can be split into three categories which include the design of a new process, new production capacity for a process, or modification of an existing process. After generating a design concept, fitness testing will begin which in most cases will include a computer simulation. Guidelines that engineers follow when testing a new design include providing equipment size and performance estimates, verifying that the results of simulations are reasonable, obtaining values for the approximate costs of process units, and developing preliminary process layouts. After the fitness tests have been performed, economic evaluation usually begins. During the economic evaluation step the selection and optimization of certain process criteria will occur to lower the cost of the process.

To aid process design and optimization, most chemical engineers will use diagrams to describe the plant they are working with. The three most common diagrams that are used are Block Flow Diagrams (BFD), Process Flow Diagrams (PFD), and Process & Instrumentation Diagrams (P&ID). Block Flow Diagrams are the simplest diagram and focus on the main operation sections of a given process. A BFD outlines the desired inputs and outputs for each section of the process and usually contains a preliminary mass balance. Process Flow Diagrams are the most commonly used diagrams by a chemical engineer. When constructing a PFD they usually contain all major equipment, estimate operating conditions, stream tables, utilities, and an energy/mass

balance. At this stage in the process of constructing a new process model, simulations are usually brought in to assist with calculations and an economic evaluation is performed to determine the profitability of the plant. The last and most detailed diagrams is the P&ID. A Process and Instrumentation Diagram includes everything from a PFD and sensor information, controls/controllers, equipment dimensions, utility connections, and the location of the equipment within the plant. P&IDs are very detailed and are mostly used for reference within a plant. PFDs are much more common because they are not so detailed.

After a process has been designed, the next step will be process optimization. Optimization is defined as the process of improving an existing system such as a chemical process. When optimizing, there are independent variables known as decision/design variables that are usually under control of an engineer. These variables could include temperature and pressure within the process or the number of trays within a column. Constraints are what limits the decision variables and can include more than one constraint. There are two types of optimum that can be found: global optimum and local optimum. The global optimum is the point at which the objective function is the best for all of the variables [1]. A local optimum is the point at which one point is the best for a small number of variables. Discrete optimization is the process of finding local optimum for several different points of the process.

The two types of optimization are topological and parametric optimization. Topological optimization looks at the arrangement of process equipment and parametric optimization looks at parameters such as the temperature and pressure of the process. When looking at the topology of a process an engineer needs to see if by-products can be

eliminated, equipment can be eliminated or moved, separation/reaction processes can be changed, and if heat integration can improve. Parametric optimization looks at several factors including operating conditions of the reactor, single pass conversion in the reactor, recovery of unused reactants, recycle stream ratios, purity of the final product, reflux ratios, and the operating pressure of separation equipment.

When optimizing there are two strategies that can be followed and they are the top down and bottom up method. Using the top down method looks at the big picture first. After the big picture has been assessed then you begin to look at the minute details that the process involves. When using the bottom up method you begin by looking at a detailed studies and then move to the big picture. During our project we used a combination of these two methods.

These steps that have been laid out are some of the ways that are best to design and optimize a chemical process. Throughout our design project we used several of the methods that have been stated in the previous paragraphs.

II. Introduction

Landshark Inc. is considering implementing a styrene production process at its OM petrochemical facility. The proposed process utilizes the dehydrogenation of ethylbenzene to produce 100,000 tonnes of styrene per year with at least 99.5 weight percent purity. Landshark Inc. will sell the styrene to manufacturers interested in polymerizing it to make polystyrene packaging and foam insulation, which could potentially be profitable.

Our engineering team received a preliminary design and instructed to first complete a base case analysis and determine economic feasibility. We found that the plant had a net present value (NPV) of -$320.3 M. Because this NPV is negative, our team will require information about the other sections of the plant (such as a styrene polymerization section, if it exists) to make an accurate recommendation regarding the project. Assuming a later section of the OM facility does polymerize 100,000 tonnes of styrene per year, the NPV based on buying the styrene at market value is -$1.4 B; therefore, under these conditions, Landshark Inc. should pursue the project further. If Landshark Inc. does not polymerize styrene, though, they should not pursue the project further with the current design as it would only increase company debt.

After completing base case work, we then investigated changes proposed by management as well as other optimizations as we saw fit. These changes gave the plant an NPV of $31 M, which indicates that the updated design can turn a profit and the project should undergo further consideration regardless of whether or not the OM facility polymerizes styrene.

III. Base Case

Our engineering team modeled the base case of Landshark, Inc.'s preliminary design in Microsoft Excel. We simulated the same design in Pro/II to utilize more complicated and realistic thermodynamic relationships in our calculations. We then compared those results to theExcel simulation, which assumed that the streams behave as ideal gases and solutions. In Pro/II, we used the SRK-SimSci thermodynamic model based on the path our system follows in the thermodynamic flowsheet (see Appendix

A11). The tower T-502 scheme, however, was simulated using the ideal thermodynamic method.

Our team found that the preliminary design as given to us by management had a NPV of -$320.3 M and an annual equivalent (AE) of -$51.7 M with a 12% minimum acceptable rate of return (MARR). This results in both a conventional and a discounted payback period greater than 12 years. Because the project had a negative NPV and a payback period longer than the project life, the project is not profitable with the preliminary design. However, with changes it could become more economically reasonable.

After inspection, several process parameters in the base case fell outside of normal operating conditions defined in *Analysis, Synthesis, and Design of Chemical Processes* by Turton et al. We then analyzed whether each of these conditions was justified. First, moving sequentially through the plant, reactors R-501 and R-502 had both high temperature and non-stoichiometric feed. This is justified because the steam present in the feed improves reactor conversion and provides heat to both fuel the reaction and keep all components in the gas phase. The low pressure of the towers T-501 and T-502 and the vessels V-502 and V-503 is justified by the need of a gas phase for vapor-liquid equilibrium and the lack of pumps or valves between the towers and vessels. The large log mean temperature differences of heat exchangers E-501, E-502, E-503, and E-505 is justified because the utilities defined in the base case (either high pressure steam or cooling water) is required to vaporize or cool each exchanger's respective stream. Compressor C-501 also has a pressure ratio of 6; however, unlike the previous parameters, this is not justified and must be changed for the optimized case.

Finally, we utilized sensitivity analysis (shown in Appendix B1) to determine which parameters had the greatest effect on NPV. As can be seen in the figure, the styrene price and the raw materials cost varied the most. Due to this observation, we decided to focus on reducing the raw materials cost.

IV. Notes about Sign Conventions for Optimization

The engineering team used discrete optimization when trying to make improvements to the styrene production process. When referring to an increased cost, the NPV contribution is becoming more negative.

V. First Change: Reactor Type

The first change we investigated was replacing the original isothermal reactors with adiabatic reactors. We treated the Isothermal Reactors as heat exchangers, since the reacting stream will only undergo a pressure drop within the reactor. We treated Adiabatic Reactors as vessels, since the reacting stream will undergo both a temperature and a pressure drop within the reactor. Ultimately, the objective in doing this was to decrease the raw materials cost by increasing the overall yield of styrene.

Appendix B2 shows an economic comparison of the process after implementing each type of reactor. Notice that the inlet temperature of the adiabatic reactor R-503 is 25°C lower in comparison to the original isothermal reactor. This adjustment was made because preliminary design conditions stipulated that the temperature drop in each reactor must be less than 50°C. The choice of 525°C resulted in a temperature drop of 49.86°C. Lowering the temperature further would result in a lower NPV because it increases the fixed capital investment as well as the annual cost of raw materials and utilities. Overall,

these changes improved the NPV by approximately $56 M. Appendix B2 shows the breakdown of the most notable cost contributions (raw materials, utilities, and fixed capital investment).

The largest contribution to the improved NPV was the decrease in the cost of raw materials. This was due to a lower single pass conversion of ethylbenzene in the reactor section (57% to 42%), which ultimately resulted in a larger ethylbenzene recycle stream and a higher overall yield of styrene (50% to 58%). The elimination of the original isothermal reactor also increased NPV by saving approximately $2 M in heating utility costs. However, this is counteracted but not overcome by the almost 4,800 kmol/hr increase in the steam utility required to heat the reactor R-503 effluent (stream 12) to the inlet temperature of R-504.

The contribution of the FCI to the project's NPV is primarily attributed to three different points in the process. Firstly, the adiabatic reactors R-503 and R-504 have larger equipment equipment cost attributes, which are related to capacity and are reported in square meters for heat exchangers and cubic meters for vessels. In this process, the vessel volume is the same as the catalyst volume- 50 m^3- while the heat exchanger area required is smaller (and it stores the required volume of catalyst in its shell.) Therefore, the equipment with the larger equipment cost attributes (vessels) is more expensive. Second, the duty (and therefore the size) of the fired heater increased when the process implements an adiabatic reactor. This is due to the increased steam utility in heat exchanger E-503. Lastly, the cost of the tower T-502 scheme increases because the number of towers required increases from 4 to 5. This is due to the lower single pass conversion of ethylbenzene in the reactor sections; therefore, a larger amount of

ethylbenzene will be separated from the styrene in T-502, and the higher flowrate requires a larger tower volume.

Overall, this decision is based on a comparison between the preliminary isothermal reactor and the optimized adiabatic reactor. If given more time, the engineering team will pursue optimization of the isothermal reactor for a more thorough decision concerning which reactor type is preferable.

VI. Second Change: Reactor Conditions

The second change we investigated was changing the volume and pressure of reactor R-503 and the volume of R-504. Similarly to the change from isothermal to adiabatic reactors, the objective in doing this was to decrease the raw materials cost (by increasing the overall yield of styrene). Overall, these changes improved the NPV by approximately $60 M. A breakdown of the most notable cost contributions (raw materials, catalyst, utilities, and fixed capital investment) is shown in Appendix B3.

The most significant change in the reactor scheme was adjusting the volumes of R-503 and R-504 from 50 to approximately 36 m^3. In both reactors this resulted in a slight decrease in single-pass conversion and an increase in the selectivity of ethylbenzene, as seen in Appendices B4-B7. The changes in conversion and selectivity ended up increasing the yield of styrene from the reactors (from 58% to 68%). This in turn decreased the required feed of ethylbenzene by 28.4 kmol/hr, which ultimately decreased the raw materials cost by $22 M per year. Since the catalyst volume is proportional to the reactor volume, this change accompanied a decrease in the catalyst cost of $2.5 M per year.

An insignificant change made to the reactor scheme was changing the inlet pressure to R-503 from 190 to 187.5 kPa. This only increased the NPV by approximately $1 M due to the given rate law equations. Since the rate law equations use partial pressure, changing the total pressure will have little effect on the rates.

VII. Third Change: Materials of Construction

The third investigation was on the materials of construction of the towers and reactors. The preliminary tower design specified using titanium, which is very expensive. Carbon steel is usable at the towers' operating conditions (vacuum pressures and T<125°C) and is about 11% the cost of titanium. The outsides of the towers will need to be epoxied or painted to prevent atmospheric corrosion.

The base case reactors were made of 316 stainless steel which is susceptible to hydrogen embrittlement and hydrogen blistering. This is where atomic hydrogen diffuses into a dislocation in a metal and bonds with another atomic hydrogen to form a gas. The gas expands and damages equipment, causing it to need to be replaced more frequently ("Hydrogen embrittlement"). Due to the mechanism of ethylbenzene dehydrogenation, atomic hydrogen will be present in the reactors. We changed the material of construction to nickel alloy clad, which is less susceptible to hydrogen embrittlement and hydrogen blistering, since it is also operable under the reactors' conditions (T<600°C and P<200 kPa). This change slightly decreased the NPV by increasing the FCI. This occurred because nickel alloy clad is more expensive than stainless steel.

Ultimately, changing the material of construction of the towers and reactors increased our NPV by $165 M. The main contribution to this was a decrease in the FCI

because the decreased tower cost greatly outweighed the increased reactor cost. This can be found in Appendix B8.

VIII. Fourth Change: Extra Tower to Purify Benzene Stream

The fourth change that was analyzed was the addition of a benzene/toluene distillation tower (T-503). The benzene and toluene byproduct stream fed to T-503 at 50°C and 200 kPa. Tower T-503 separated the benzene and toluene and deliver benzene with 99.5 mole percent purity to the bottoms. With this high purity Landshark, Inc. could sell the benzene at full price therefore increasing the revenue of the plant from $239 M to $253 M. This outweighs the $0.5 M decrease in FCI. This ultimately increased NPV by $56 M.

IX. Fifth Change: Heat Integration

Due to the recent decrease in the market value of utilities, the engineering team only focused on implementing heat integration in one section of the process. In the preliminary design, high pressure steam (HPS) heated and vaporized stream 2 in heat exchanger E-501. The effluent from reactor R-502, or stream 12, flowed directly into heat exchanger E-503 where it was cooled through interacting with cooling water (CW) and exited as stream 13. The preliminary design PFD shows this setup (Appendix A1).

The proposed changes shown in the optimized design PFD (Appendix A5) resulted in an elimination of the HPS utility in E-501 and a reduction in the CW required in E-503. In the new design, the effluent stream 12 from reactor R-504 (previously called R-502 in the base case) redirects to the utility side of E-513 (previously E-501). Since it now serves as the heating fluid, its temperature decreases in the heat exchanger and exits

as stream 36. This flows into E-503 where it cools further to become stream 13. Overall, this improved the NPV by approximately $4 M. Appendix B9 shows the breakdown of the most notable cost contributions (raw materials, utilities, and fixed capital investment).

X. Sixth Change: Compressor Adjustments

In the base case, the pressure ratio across compressor C-501 was 6. For safe operating conditions the pressure ratio needed to be decreased to below 3. To achieve this, the engineering team looked into using multi-stage compression. When adding a second compressor (C-502) with an interstage cooler, the pressure ratio decreased to approximately 2.45 across both C-501 and C-502. We accepted this change because it is under the threshold for safe operation. With the addition of a second compressor (C-502) and a heat exchanger (E-512), the utilities and FCI decreased compared to the base case. This increased the NPV by $11 M.

XI. Summary

The economic data for the optimized case results in an NPV of $31 M, a discounted cash flow rate of return (DCFROR) of 16%, and an annual equivalent (AE) of $4.93 M. Provided below in Appendix B10 is a comparison of the optimized case and the base case. The DCFROR for the base case has been marked as N/A since it could not be calculated.

XII. Process Safety Considerations

Overall, one of the main concerns for process safety will be keeping high temperature vapors and steam away from employees. If exposure to high temperature lines is likely maintenance staff/operators should wear proper PPE. Otherwise, during

the design process engineers can protect employees by consciously attempting to put high temperature process and steam lines away from expected high traffic areas. In addition, the temperatures throughout the process are higher than the flash points of each component. Therefore, there will need to be measures put into place to avoid ignition sources. Also, since the reaction is endothermic, runaway reactions will not be a concern. However, isolating the reactors, where temperatures of the streams are extremely high, would also be advisable. This alleviates the danger of burns if there is a rupture in piping or equipment.

The other main process safety concern noted was limiting exposure to the chemicals in the process. In the case of a spill, people should self-contained respiratory device as high concentrations of chemical vapor as the components in the process can act as lung irritants and asphyxiants. Also, proper ventilation should be in place in all areas where spills are likely to occur.

XIII. Sensitivity Scenarios

The three parts of this process that were most susceptible to change were the prices of ethylbenzene, styrene, and utilities; therefore, the team focused on formulating scenarios for changes in these variables. The following changes would affect the optimized case defined above.

First, the team investigated ethylbenzene and styrene scenarios. If the price of ethylbenzene decreases, then the team would not have to focus so much on maximizing the overall yield of styrene. Also, if the price of ethylbenzene increases or the price of styrene decreases, it might not be profitable to produce the styrene. It may be better to

simply purchase the styrene. Lastly, if the price of styrene increases, the profitability of producing the styrene on-site would increase.

In addition, utility costs are susceptible to change. If the cost of utilities were to increase, heat integration would need further investigation and implementation. This would allow the plant minimize the amount of utilities. If the cost of utilities were to go down, little would change in the optimized design process.

XIV. Conclusions from Original Case

The engineering team determined the economic viability of producing styrene from the dehydrogenation of ethylbenzene given specifications of 100,000 tonnes of styrene produced per year with a purity of at least 99.5 wt%. The NPV of the base case was -$320.2 M.

However, after the proposed changes, the NPV of the optimized case was $31 M. Therefore we recommend the optimized case undergo further development and optimization. Our recommendations include investigating different inlet temperatures and pressures in tower T-503, adding more heat integration, and improving vessel V-501. After finishing optimization, Landshark Inc. could begin to discuss options for buying the process equipment from contractors, thus reducing the design inaccuracy due to the pricing calculations.

XV. Introduction of Fluidized Bed Reactor and Calculation Methods

After completing the original case we were tasked with calculating the effects of a fluidized bed reactor (FBR) on the styrene production process to fulfill the requirements of the Sally McDonnell Barksdale Honors College Senior Thesis. Fluidized

bed processes have been used since the 1920s in industry. They have been used in many different fields including coal gasification, fluidized catalytic cracking and almost 75% of all polyolefins today are made using this process. Fluidized beds can be more complex to design and build than other reactors and scale-up of a fluidized bed reactor can be very difficult. While they do have their challenges, fluidized beds do offer some distinct advantages. Within a fluidized bed reactor there is usually better heat transfer, the particle size distribution varies heavily, and it is much easier to move solids like a fluid through the reactor. The fluidized bed can often offer up to 10 times more heat transfer than the standard packed bed reactor. [3]

When simulating a fluidized bed reactor, an isothermal plug flow reactor can be used. While it is able to maintain the temperature within a few degrees to make it isothermal, it does require a heat exchanger to supply the amount of heat lost. Also, to design this you must only use 90% of the feed in your calculations for the reactor because a fraction of the gas will not react even in the largest FBR. One constraint when using a FBR is that the catalyst has a temperature range of less than 1000 K.

Some information was provided with the problem statement for the fluidized bed reactor. The first specification was the diameter of the catalyst particles. They were said to be nearly spherical and approximately 300 micrometers in diameter. The void fraction for the new catalyst is 0.45 compared to the 0.5 void fraction used on the original project. Because of this we are able to pack the catalyst in more efficiently. Some other specifications included were for the heat transfer tubes. The tubes are 25 mm in diameter and 20 ft. long. The overall heat transfer coefficient for the tubes is 200 $W/m^{2}°C$. It will

cost approximately \$10,000 per m^2 of heat transfer surface for the installed cost of the reactor. The bare module factor (C^o_{BM}) is 2.5.

When beginning calculations, we replaced the isothermal packed bed reactors and the adiabatic packed bed reactors with a fluidized bed reactor on their respective Excel simulation sheets. Once the numbers and assumptions given in the process statement were inserted we were able to begin the calculations on the FBR. We assumed that there was one large reactor with a volume of 250 m^3. Just as we had done on the previous reactors, the calculations were split into 10 intervals of cubic meters.

After setting up the Excel sheet, we began the rigorous calculations for the FBR. The first step was to calculate the change in moles of each component using the four rate laws shown in Appendix C1. Moles of water were held constant in these calculations because there was steam present. Next, we calculated the pressure drop using the Ergun equation. Because length and area of the reactor were not originally known they had to be calculated and they varied with each of the 10 intervals.

To find the reactor length we first needed to find the superficial gas velocity and also determine the cross sectional area of the reactor. To find the superficial gas velocity (μ_g), you must use the Reynolds and Archimedes number formulas. We had the information needed for these formulas and were able to solve and then multiply it by a factor. This factor lies between 3-10 times the minimum fluidization velocity. We chose 6.5 because it is the median of that range.

We then determined the cross sectional area using the volumetric flowrate (from the Ideal gas law) and the superficial gas velocities calculated for each interval. We then chose the last interval to represent our cross sectional area and superficial velocity.

After performing the calculations, the FBR had a cross sectional area of 198 m^2 and a length of 1.3 m with a pressure drop of 56.5 kPa. The large cross sectional area caused us to remedy this by splitting it into two fluidized bed reactors. When there are two reactors, each would have a volume of 125 m^3 and a diameter of 11.2 m. This makes it more reasonable in size. The reactors would still have 100 tubes.

The final step of our process was to simulate the fluidized bed reactor using Pro/II software. This simulation can be found in Appendix C5. The component flowrates out of the simulated reactor were very close in comparison to our Excel simulation.

XVI. Comparing Reactors Based on EAOCs

To compare the reactor types and determine which would be the best we calculated the estimated annual operating costs for each type of reactor. Before we could determine the EAOC we first had to find the annual equivalent of the capital investment shown in the formula below.

$$A = P\left[\frac{i(1+i)^N}{(1+i)^N - 1}\right]$$

The N (plant life) is 12 years and the i (interest rate) is 12%. For the isothermal reactor we compared it against the fluidized bed reactor at the base case numbers. Since we optimized the adiabatic reactor, we compared the FBR against it at the optimized case. The results are shown in Table 1 and Table 2 below.

Table 1: Isothermal vs FBR

EAOC of Reactor in the Base Case Styrene Process	
Isothermal	$9,736,000
Fluidized Bed	$4,620,000

Table 2: Adiabatic vs. FBR

EAOC of Reactor in the Optimized Styrene Process	
Adiabatic	$18,466,000
Fluidized Bed	$8,753,000

Once the EAOC was completed for the FBR we were not able to optimize further because the EAOC was only affected by the number of tubes and to keep our calculations more accurate we left the number of tubes at 100.

Based on the EAOC calculations, it is obvious that the fluidized bed reactor was the best option to minimize the cost of the reactor. Because the FBRs have more efficient heat transfer and do not require as many reactors, it becomes clear that the FBR should be the choice for this process. Because of time requirements we were not able to check into optimizing the FBR, but that would be what would come next in the design and optimization process.

XVII. Appendix A

1. Base Case PFD

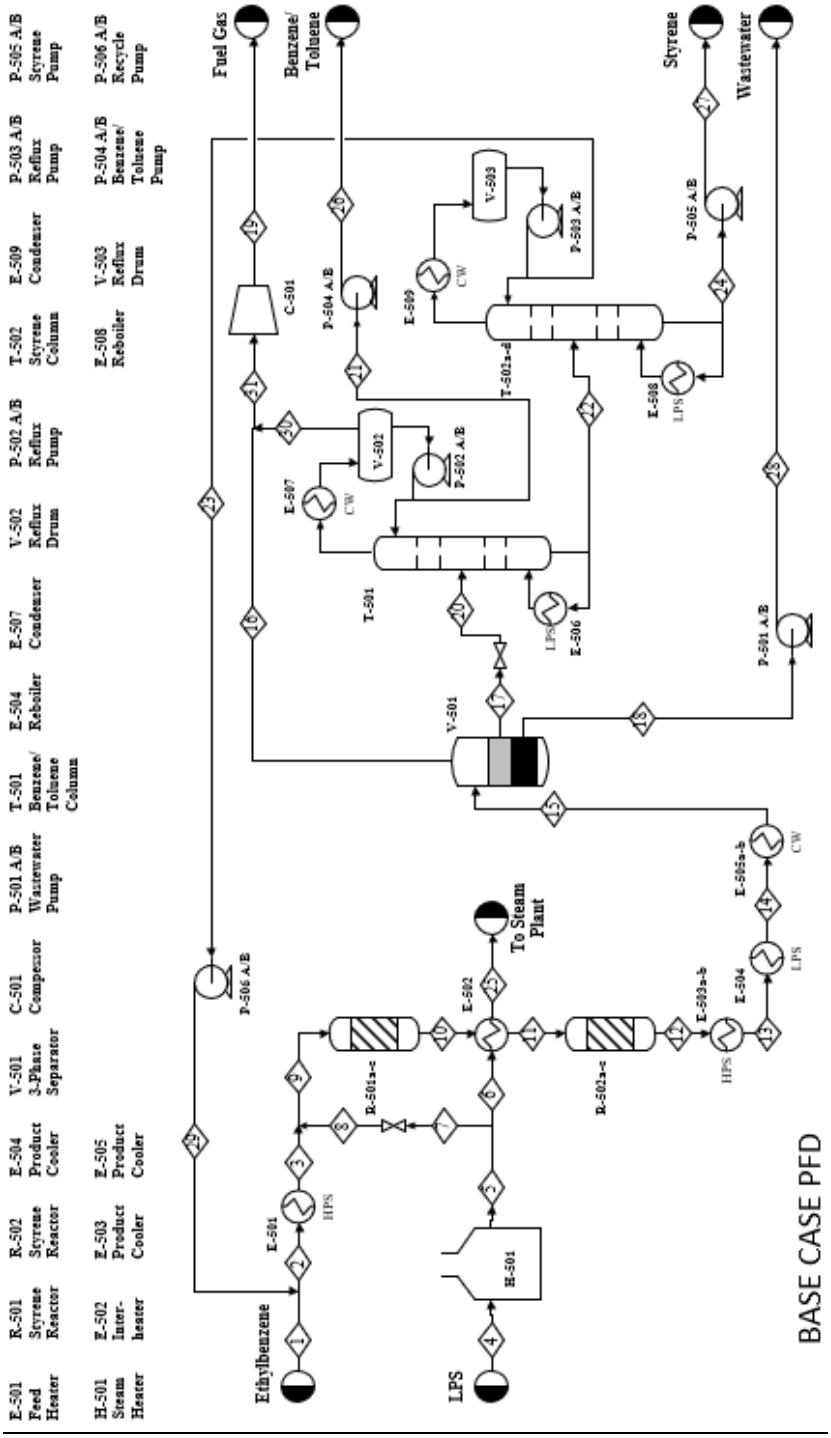


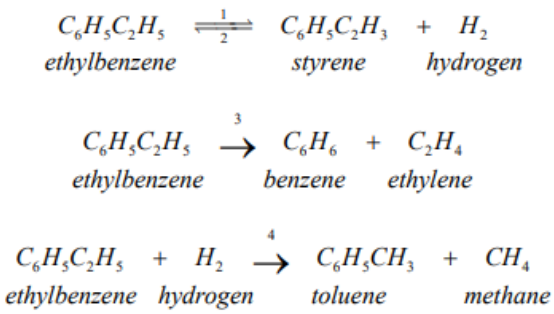
Figure 1: Base Case Process Flow Diagram Provided in Problem Statement

2. Base Case Stream Table

Stream No.	1	2	3	4	5	6	7	8	9
Temperature (°C)	136	117	225	159	800	800	800	800	550
Pressure (kPa)	205	205	190	600	565	565	565	190	190
Vapor Mole Fraction	0	0	1	1	1	1	1	1	1
Total Flow (kg/h)	26430	45962	45962	90742	90742	28288	62454	62454	108416
Total Flow (kmol/h)	250	434	434	5037	5037	1570	3467	3467	3901
Comp. Flow (kmol/h)									
Water	0	0	0	5037	5037	1570	3467	3467	3467
Ethylbenzene	245	427	427	0	0	0	0	0	427
Styrene	0	1.2	1.2	0	0	0	0	0	1.2
Hydrogen	0	0	0	0	0	0	0	0	0
Benzene	2.5	2.5	2.5	0	0	0	0	0	2.5
Toluene	2.5	3.1	3.1	0	0	0	0	0	3.1
Ethylene	0	0	0	0	0	0	0	0	0
Methane	0	0	0	0	0	0	0	0	0
Stream No.	10	11	12	13	14	15	16	17	18
Temperature (°C)	550	575	575	270	180	65	65	65	65
Pressure (kPa)	180	165	147	132	117	102	102	102	102
Vapor Mole Fraction	1	1	1	1	1	0	1	0	0
Total Flow (kg/h)	108416	108416	108416	108416	108416	108416	3738	43077	61600
Total Flow (kmol/h)	4023	4023	4080	4080	4080	4080	219	442	3419
Water	3467	3467	3467	3467	3467	3467	47	0	3419
Ethylbenzene	273	273	186	186	186	186	0.9	185	0
Styrene	98	98	121	121	121	121	0	121	0
Hydrogen	64	64	58	58	58	58	56	1.5	0
Benzene	28	28	62	62	62	62	2.1	60	0
Toluene	35	35	65	65	65	65	0.8	64	0
Ethylene	25	25	60	60	60	60	51	8.4	0
Methane	32	32	62	62	62	62	59	2.7	0
Stream No.	19	20	21	22	23	24	25	26	27
Temperature (°C)	227	65	50	121	91	123	700	50	123
Pressure (kPa)	240	60	40	60	25	55	555	200	200
Vapor Mole Fraction	1	0	0	0	0	0	1	0	0
Total Flow (kg/h)	5354	43077	9430	32032	19532	12500	28288	9430	12500
Total Flow (kmol/h)	247	442	110	304	184	120	1570	110	120
Water	47	0	0	0	0	0	1570	0	0
Ethylbenzene	1.0	185	1.8	183	182	0.6	0	1.8	0.6
Styrene	0	121	0	121	1.2	119	0	0	119
Hydrogen	58	1.5	0	0	0	0	0	0	0
Benzene	14	60	49	0	0	0	0	49	0
Toluene	5.5	64	59	0.6	0.6	0	0	59	0
Ethylene	59	8.4	0	0	0	0	0	0	0
Methane	62	2.7	0	0	0	0	0	0	0
Stream No.	28	29	30	31					
Temperature (°C)	65	91	50	63					
Pressure (kPa)	200	205	40	40					
Vapor Mole Fraction	0	0	1	1					
Total Flow (kg/h)	61600	19532	1615	5354					
Total Flow (kmol/h)	3419	184	29	247					
Water	3419	0	0	47					
Ethylbenzene	0	182	0	1.0					
Styrene	0	1.2	0	0					
Hydrogen	0	0	1.5	58					
Benzene	0	0	11	14					
Toluene	0	0.6	4.7	5.5					
Ethylene	0	0	8.2	59					
Methane	0	0	2.7	62					

3. Base Case Process Description

Fresh liquid ethylbenzene at 136°C and 205 kPa (stream 1) is combined with a recycle of liquid ethylbenzene (stream 29) to form a feed mixture (stream 2). This then enters heat exchanger E-501 which utilizes high pressure steam to vaporize the stream and increase its temperature to 225°C (stream 3). The stream experiences a pressure drop of 15 kPa through the heat exchanger, which is typical of all of the heat exchangers in the process. The vaporized stream 3 is mixed with an adequate amount of high pressure steam (stream 8) to form stream 9. This stream is then fed to reactor R-501a-e at a temperature of 550°C and a pressure of 190 kPa. The reactor consists of a catalytic bed and has 4 reactions that occur:



The effluent (containing ethylbenzene, styrene, hydrogen, benzene, ethylene, toluene and methane) coming from the reactor at 550°C and 179.9 kPa (stream 10) is then sent to a heat exchanger E-502 that increases the temperature to 575°C. Stream 11 coming from E-502 enters the second reactor R-502a-e and undergoes the same reactions shown previously. The 8-component vapor stream exiting the reactor (stream 12) is fed to a series of three heat exchangers (E-503, E-504, and E-505, which use high pressure steam, low pressure steam, and cooling water utilities respectively). Here the vapor is cooled and partially condensed into a liquid/vapor mixture at 65°C and 102.2 kPa (stream

15.) This mixture is then fed to a 3-phase separator, V-501, where it separated into three streams: the vapor stream (stream 16), containing all the aqueous and organic components in the inlet stream, the organic liquid stream (stream 17), and a water stream (stream 18). The vapor stream is mixed with the fuel gas coming out of reflux drum V-502 (stream 30) to form stream 31. Stream 31 is then fed to compressor C-501 which increases the temperature and pressure to 227°C and 240 kPa (stream 19). These are the conditions at which the stream is sold as fuel gas. The water stream is fed to pump P-501A/B where the pressure is increased to 200 kPa and treated as wastewater. The organic liquid stream goes through a valve and comes out at 60 kPa (stream 20). Stream 20 is then fed onto tray 4 of the first tower T-501, which has 18 stages and operates at 65° C and between 40 and 60 kPa. This tower has a reboiler, E-506, which uses a low pressure steam utility. The column produces a bottoms stream (stream 22) which recovers 1% of the toluene and 99% of ethylbenzene in stream 20.

The vapor stream from the top of T-501 is condensed in heat exchanger E-507 using cooling water and sent to Reflux Drum V-502. Here the vapor and liquid phases are separated into streams 30 and 21 respectively. The vapor stream 30 is combined with the fuel gas. The liquid benzene/toluene byproduct (stream 21) is sent to pump P-504A/B where the pressure is increased to 200 kPa. Stream 22 (bottoms product from T-501) is fed to tray 28 of T-502 where further separation is accomplished. T-502 contains 68 total stages, and it operates between 25 and 55 kPa. It also has a reboiler (E-508), which uses low pressure steam. The vapor product from the top of the T-502 condenses in heat exchanger E-509, using cooling water, before it goes through reflux drum V-503. The liquid stream then goes through pump P-503A/B where its pressure decreases to 25

kPa (stream 23). Stream 23 is then sent through P-506A/B where the pressure is increased to 205 kPa before it is recycled and combined with stream 1. The bottoms of T-502 in stream 24 are sent to P-505A/B where it undergoes a pressure increase to 200 kPa to become stream 27. This is the final pure styrene product (with a 99.5 mass percent purity) flowing at a rate of 100,000 tonnes per year.

The only other inlet stream is low pressure steam fed to the fired heater H-501 at 159°C and 600 kPa (stream 4). It is heated in H-501 to 800°C in stream 5 where it is then split into streams 6 and 7. Stream 7 goes through a valve where there is a 375 kPa pressure drop before going into stream 8 which combines with stream 3. Stream 6 is fed to heat exchanger E-502 and is used to heat the first reactor effluent (stream 10) to 575°C.

4. Optimized Case Process Description

Fresh liquid ethylbenzene at 136°C and 205 kPa (stream 1) is combined with a recycle of liquid ethylbenzene (stream 29) to form a feed mixture (stream 2). This then enters heat exchanger E-513 which utilizes stream 12 from reactor to vaporize the stream and increase its temperature to 225°C (stream 3). The stream experiences a pressure drop of 15 kPa through the heat exchanger, which is typical of all of the heat exchangers in the process. The vaporized stream 3 is mixed with an adequate amount of high pressure steam (stream 8) to form stream 9. This stream is then fed to reactor R-503a-e at a temperature of 525°C and a pressure of 187.5 kPa. The reactor consists of a catalytic bed and has 4 reactions that occur:

The effluent (containing ethylbenzene, styrene, hydrogen, benzene, ethylene, toluene and methane) leaves the reactor at 483°C and 164 kPa (stream 10). It is then sent to heat exchanger E-502 where the temperature increases to 575°C. Stream 11 coming from E-502 enters the second reactor, R-504a-e, and undergoes the same reactions shown previously. An 8-component vapor stream exits the reactor (stream 12) and is then used as the utility in E-513. Stream 12 goes through E-513 and become stream 36 which is fed to a series of three heat exchangers (E-503, E-504, and E-505, which use high pressure steam, low pressure steam, and cooling water utilities respectively). Here the vapor is cooled and partially condensed into a liquid/vapor mixture at 65°C and 68 kPa (stream 15). This mixture is then fed to a 3-phase separator, V-501, where it separated into three streams: the vapor stream (stream 16), containing all the aqueous and organic components in the inlet stream, the organic liquid stream (stream 17), and a water stream (stream 18). The vapor stream is mixed with the fuel gas coming out of reflux drum V-502 (stream 30) to form stream 31. Stream 31 is then fed to compressor C-501 which increases the temperature and pressure to 157°C and 98 kPa (stream 34). Stream 34 is sent to an interstage cooler E-512 where it cools the stream to 63°C (stream 35). Stream 35 is then fed to compressor C-502 where its temperature and pressure are increased to 157°C and 240 kPa (stream 19). These are the conditions at which the stream is sold as fuel gas in stream 19. The water stream (stream 18) is fed to pump P-501A/B where the pressure is increased to 200 kPa and treated as wastewater. The organic liquid stream goes through a valve and comes out at 60 kPa (stream 20). Stream 20 is then fed to tower T-501 which has 32 stages and operates at 65°C and between 40 and 60 kPa. This tower has a reboiler, E-506, which uses a low pressure steam utility. The column produces a

bottoms stream (stream 22) which recovers 1% of the toluene and 99% of ethylbenzene in stream 20.

The vapor stream from the top of T-501 is condensed in heat exchanger E-507 using cooling water and sent to Reflux Drum V-502. Here the vapor and liquid phases are separated into streams 30 and 21 respectively. The vapor stream 30 is combined with the fuel gas. The liquid benzene/toluene byproduct (stream 21) is sent to pump P-504A/B where the pressure is increased to 200 kPa (stream 26). Stream 26 is then fed to tower T-503 where the overhead product (Stream 32) is 99.5 mole % benzene. The overhead is condensed in exchanger E-511 and sent to Reflux Drum V-504. After V-504 the stream is sent through pump P-507A/B where stream 32 is sold as benzene. The bottoms for T-503 is the Toluene stream in stream 33 that is sold. The reboiler for tower T-503 is E-510. Stream 22 (bottoms product from T-501) is fed to tray 28 of T-502 where further separation is accomplished. T-502 contains 68 total stages, and it operates between 25 and 55 kPa. It also has a reboiler (E-508), which uses low-pressure steam. The vapor product from the top of T-502 condenses in heat exchanger E-509, using cooling water, before it goes through reflux drum V-503. The liquid stream then goes through pump P-503A/B where its pressure decreases to 25 kPa (stream 23). Stream 23 is then sent through P-506A/B where the pressure is increased to 205 kPa before it is recycled and combined with stream 1. The bottoms of T-502 in stream 24 are sent to P-505A/B where it undergoes a pressure increase to 200 kPa to become stream 27. This is the final pure styrene product (with a 99.5 mass percent purity) flowing at a rate of 100,000 tonnes per year.

The only other inlet stream is low pressure steam fed to the fired heater H-501 at 159°C and 600 kPa (stream 4). It is heated in H-501 to 800°C in stream 5 where it is then split into streams 6 and 7. Stream 7 goes through a valve where there is a 375 kPa pressure drop before going into stream 8 which combines with stream 3. Stream 6 is fed to heat exchanger E-502 and is used to heat the first reactor effluent (stream 10) to 575°C.

5. Optimized Case PFD

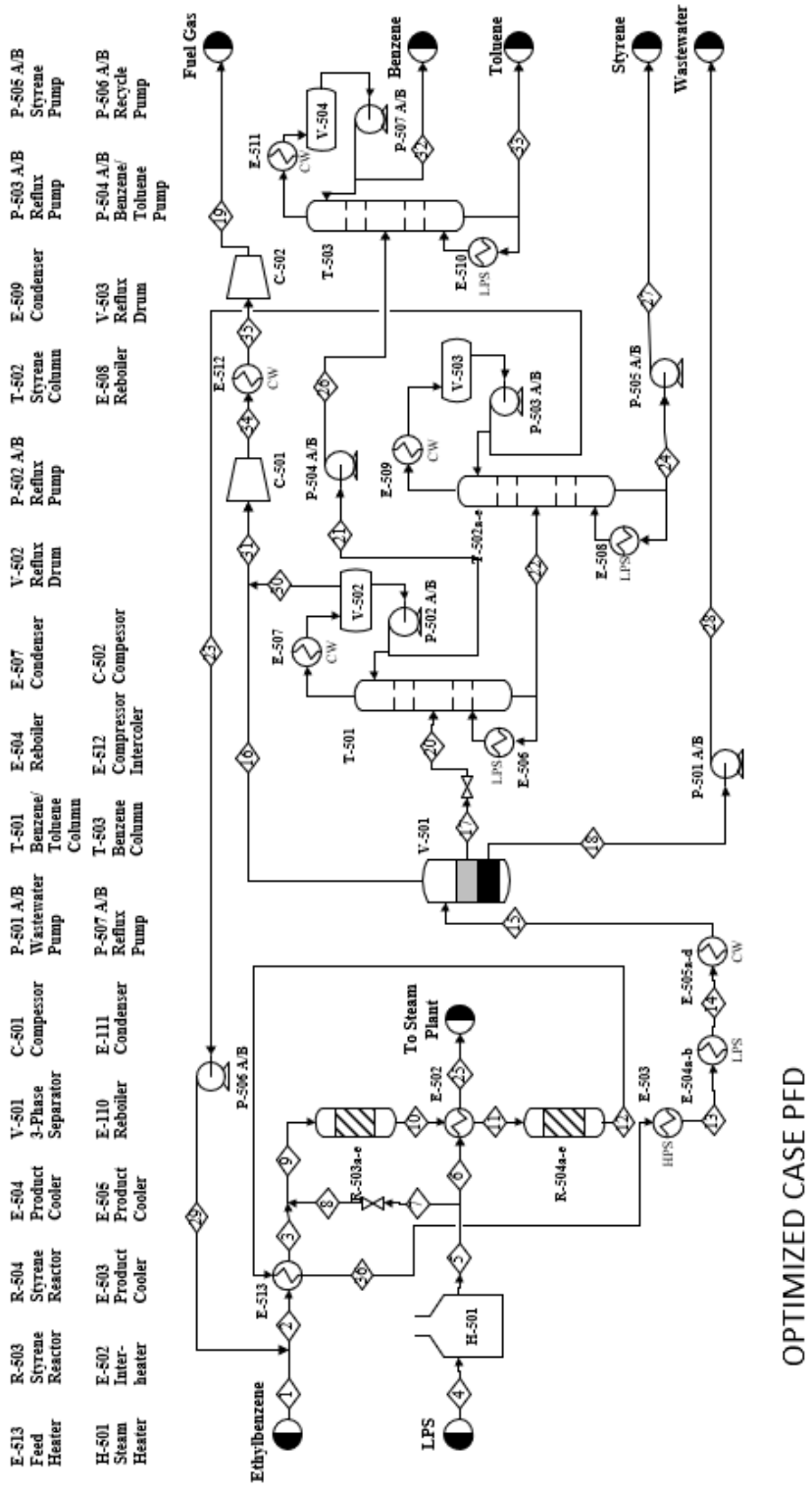


Figure 2: Optimized Case Process Flow Diagram Produced from Project Steps

6. Optimized Case Stream Table

Stream Table									
Stream No.	1	2	3	4	5	6	7	8	9
Temperature (°C)	136	107	225	159	800	800	800	800	525
Pressure (kPa)	203	203	188	600	565	565	565	188	188
Vapor Mole Fraction	0	0	1	1	1	1	1	1	1
Total Flow (kg/h)	19548	57071	57071	180973	180973	116368	64606	64606	121676
Total Flow (kmol/h)	185	538	538	10046	10046	6459	3586	3586	4125
Stream No.	10	11	12	13	14	15	16	17	18
Temperature (°C)	483	575	539	270	180	65	65	65	65
Pressure (kPa)	164	149	113	98	83	68	68	68	68
Vapor Mole Fraction	1	1	1	1	1	0	1	0	0
Total Flow (kg/h)	121676	121676	121676	121676	121676	121676	2928	55355	63393
Total Flow (kmol/h)	4190	4190	4268	4268	4268	4268	210	539	3519
Stream No.	19	20	21	22	23	24	25	26	27
Temperature (°C)	157	65	50	120	91	123	700	50	123
Pressure (kPa)	240	60	40	60	25	55	555	200	200
Vapor Mole Fraction	1	0	0	0	0	0	1	0	0
Total Flow (kg/h)	221	55355	4791	50023	37523	12500	116368	4791	12500
Total Flow (kmol/h)	3469	539	55	474	353	120	6459	55	120
Stream No.	28	29	30	31	32	33	34	35	36
Temperature (°C)	65	91	50	63	80	136	157	63	429
Pressure (kPa)	200	203	40	40	170	190	98	98	113
Vapor Mole Fraction	0	0	1	1	0	0	1	1	1
Total Flow (kg/h)	63393	37523	541	3469	20	34	221	221	121676
Total Flow (kmol/h)	3519	353	11	221	1571	3219	3469	3469	4268

7. Optimized Case Utility Summary Table

Utility Summary for Unit 500

E-503		E-504		E-505		E-506	
bfw → hps		bfw → lps		cw		lps → bfw	
18588	kg/h	9486.927	kg/h	4739512	kg/h	10366.73	kg/h

E-507		E-508		E-509	
cw		lps → bfw		cw	
518690	kg/h	43652.02	kg/h	1642037	kg/h

E-510		E-511		E-512	
cw		lps → bfw		cw	
53053	kg/h	1060.334	kg/h	19547.29	kg/h

8. Optimized Case Equipment Summary Table

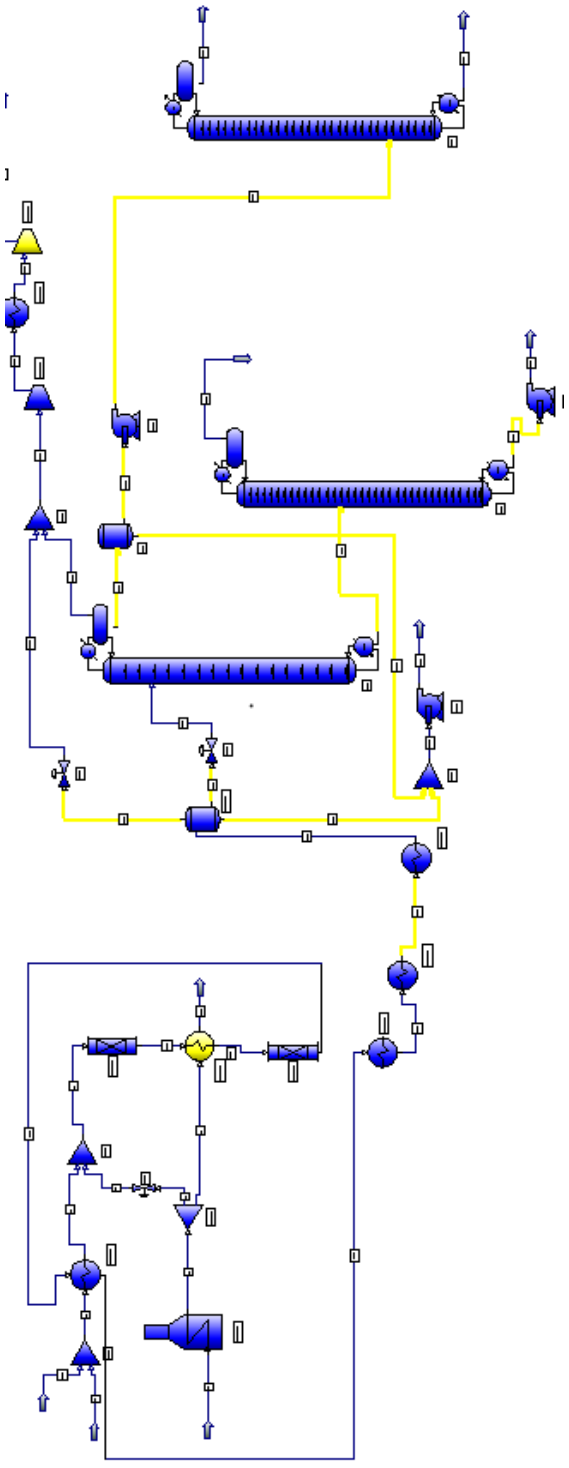
Heat Exchangers								
E-501					**E-502**			
A =	339.5187	m^2			A =	162.6254	m^2	
1-2 exchanger, fixed tube sheet, carbon steel					1-2 exchanger, floating head, 316 SS			
Process side pressure drop =		15	kPa		Process side pressure drop =		15	kPa
E-503					**E-504a-b**			
A =	1338.808	m^2			A =	474.3989	m^2	
1-2 exchanger, fixed tube sheet, 316 SS					1-2 exchanger, fixed tube sheet, carbon steel			
Process side pressure drop =		15	kPa		Process side pressure drop =		15	kPa
E-505a-d					**E-506**			
A =	419.1813	m^2			A =	177.7396	m^2	
1-2 exchanger, fixed tube sheet, 316 SS					1-2 exchanger, fixed tube sheet, 316 SS			
Process side pressure drop =		15	kPa					
E-507					**E-508**			
A =	517.4387	m^2			A =	499.8216	m^2	
1-2 exchanger, floating head, carbon steel					1-2 exchanger, fixed tube sheet, 316 SS			
E-509								
A =	471.7084	m^2						
1-2 exchanger, floating head, carbon steel								

Pumps							
P-501 A/B				**P-502 A/B**			
Carbon Steel - centrifugal				Carbon steel - centrifugal			
Actual power =	2.263131	kW		Actual power =	3.450626	kW	
Efficiency =	0.75			Efficiency =	0.75		
Electric Drive				Electric Drive			
P-503 A/B				**P-504 A/B**			
Carbon Steel - centrifugal				Carbon steel - centrifugal			
Actual power =	23.19948	kW		Actual power =	0.643176	kW	
Efficiency =	0.75			Efficiency =	0.75		
Electric Drive				Electric Drive			
P-505 A/B				**P-506 A/B**			
Carbon Steel - centrifugal				Carbon steel - centrifugal			
Actual power =	0.742584	kW		Actual power =	1.504448	kW	
Efficiency =	0.75			Efficiency =	0.75		
Electric Drive				Electric Drive			

Fired Heater			
H-301			
Fired heater - refractory lined, stainless steel tubes			
Required heat load =	123309.8	MJ/h	
Design (maximum) heat load =	164.413	GJ/h	
Thermal Efficiency =	0.75		

Compressors and Drives									
C-501					**D-401 A/B**				
Carbon steel					Electric/explosion proof				
W =	538.1611	kW			W =	717.5481	kW		
Adiabatic Efficiency =		0.75			Efficiency =		0.98		
Pumps									
P-501 A/B					**P-502 A/B**				
Carbon Steel - centrifugal					Carbon steel - centrifugal				
Actual power =		2.263131	kW		Actual power =		3.450626	kW	
Efficiency =		0.75			Efficiency =		0.75		
Electric Drive					Electric Drive				
P-503 A/B					**P-504 A/B**				
Carbon Steel - centrifugal					Carbon steel - centrifugal				
Actual power =		23.19948	kW		Actual power =		0.643176	kW	
Efficiency =		0.75			Efficiency =		0.75		
Electric Drive					Electric Drive				
P-505 A/B					**P-506 A/B**				
Carbon Steel - centrifugal					Carbon steel - centrifugal				
Actual power =		0.742584	kW		Actual power =		1.504448	kW	
Efficiency =		0.75			Efficiency =		0.75		
Electric Drive					Electric Drive				
Fired Heater									
H-301									
Fired heater - refractory lined, stainless steel tubes									
Required heat load =		123309.8	MJ/h						
Design (maximum) heat load =			164.413	GJ/h					
Thermal Efficiency =		0.75							

9. Optimized Case Pro/II



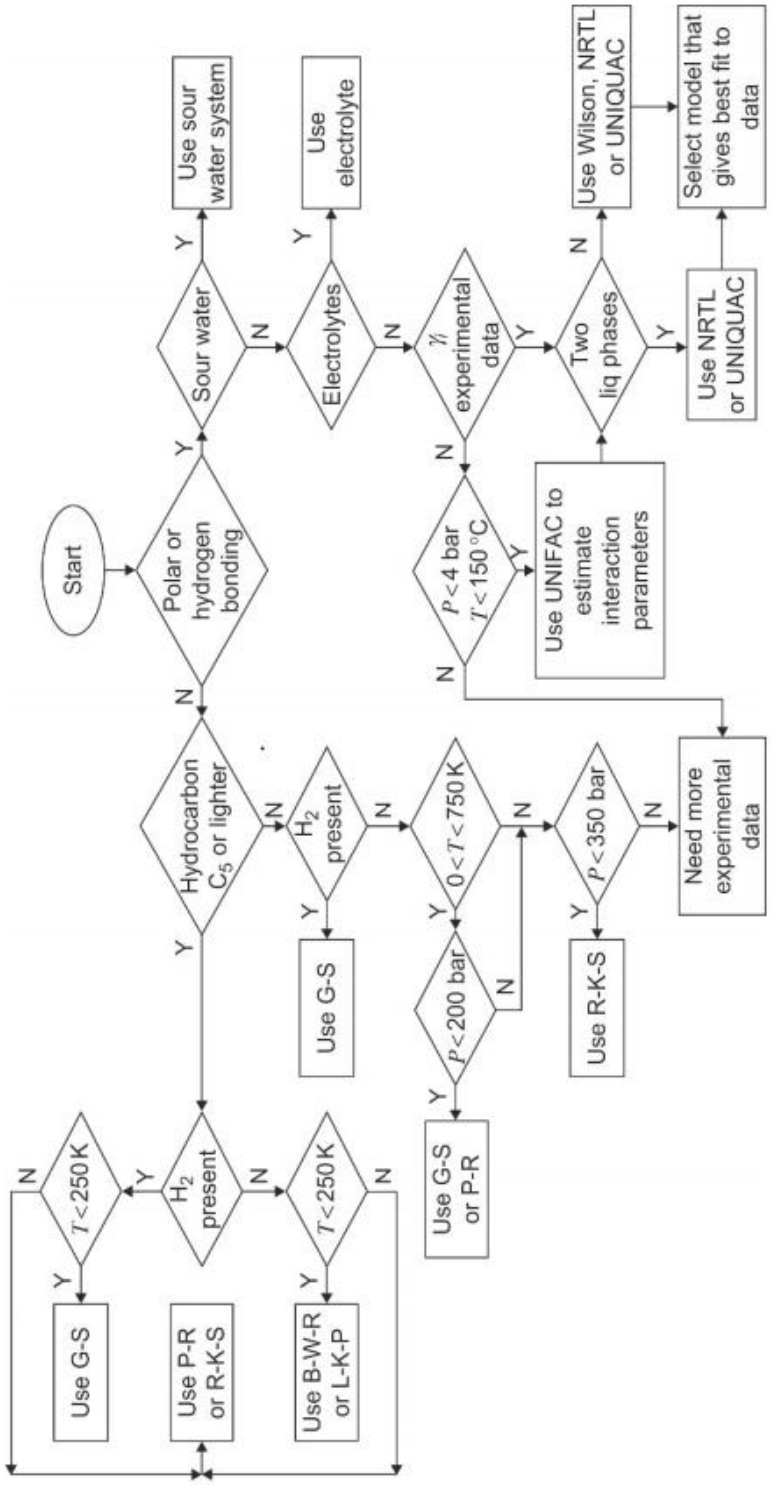
10. Optimized Case Income/Cash Flow Statement\

Income and Cash Flow Statement
(Syverne Case Key Spring 2018)

End of Year	N	2018 -2	2019 -1	2020 0	2021 1	2022 2	2023 3	2024 4	2025 5	2026 6	2027 7	2028 8	2029 9	2030 10	2031 11	2032 12
Income Statement																
Depreciation																
Land (BV)		5,000,000	5,000,000	5,000,000	5,000,000	5,000,000	5,000,000	5,000,000	5,000,000	5,000,000	5,000,000	5,000,000	5,000,000	5,000,000	5,000,000	5,000,000
Building		-	-	-	(76,923)	(76,923)	(76,923)	(76,923)	(76,923)	(76,923)	(76,923)	(76,923)	(76,923)	(76,923)	(76,923)	(73,718)
Bldg BV		-	1,500,000	3,000,000	2,926,282	2,849,359	2,772,436	2,695,513	2,618,590	2,541,667	2,464,744	2,387,821	2,310,898	2,233,975	2,157,052	2,083,334
	Bldg Dep Factor				2.4573%	2.5641%	2.5641%	2.5641%	2.5641%	2.5641%	2.5641%	2.5641%	2.5641%	2.5641%	2.5641%	2.4573%
Machines		-	-	-	(14,647,107)	(25,102,005)	(17,827,075)	(12,802,125)	(9,153,161)	(9,142,911)	(9,153,161)	(4,571,455)	-	-	-	-
Mach BV		-	68,332,667	102,499,000	87,851,893	62,749,888	44,922,813	32,020,688	22,867,527	13,724,616	4,571,455	0	-	-	0	0
	Machine Dep Factor				14.29%	24.49%	17.49%	12.49%	8.93%	8.92%	8.93%	4.46%	0.00%	0.00%	0.00%	0.00%
	Tools	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Taxable Income					20,423,259	9,849,575	16,899,276	21,895,241	25,411,350	25,284,759	25,133,563	29,570,094	33,992,020	33,838,005	33,679,369	33,518,179
Income Taxes	35%				(7,150,241)	(3,447,351)	(5,914,747)	(7,663,334)	(8,893,973)	(8,849,666)	(8,796,747)	(10,349,533)	(11,897,207)	(11,843,302)	(11,787,779)	(11,731,713)
Net Income					13,273,018	6,402,224	10,984,530	14,231,906	16,517,378	16,435,094	16,336,816	19,220,561	22,094,813	21,994,703	21,891,590	21,787,467
Cash Flow Statement																
Operating Activities																
Net Income					13,273,018	6,402,224	10,984,530	14,231,906	16,517,378	16,435,094	16,336,816	19,220,561	22,094,813	21,994,703	21,891,590	21,787,467
Depreciation					14,720,825	25,178,928	18,003,998	12,873,048	9,230,084	9,219,834	9,230,084	4,648,378	76,923	76,923	76,923	73,718
Investment Activities																
Land		(5,000,000)														3,000,000
Buildings			(1,500,000)	(1,500,000)												1,000,000
Machines (FCI or Cap. ex buildings and land)			(68,332,667)	(34,166,333)												10,243,900
Tools		-	-	-												-
Gains Tax																
Land																(1,400,000)
Buildings																379,167
Machines																(3,587,465)
Tools																-
Working Capital				(23,828,262)												23,828,262
Net Cash Flow		(5,000,000)	(69,832,667)	(59,494,595)	27,993,843	31,581,152	28,988,528	27,110,955	25,747,461	25,654,927	25,566,900	23,868,940	22,171,736	22,071,626	21,968,513	63,494,382
Cumulative Cash Flow		(5,000,000)	(74,832,667)	(134,327,262)	(106,327,418)	(74,746,267)	(45,757,739)	(18,646,784)	7,100,677	32,755,604	58,322,504	82,191,444	104,363,180	126,434,806	148,403,319	211,897,702
PV (SIU) @ 12%		(6,272,000)	(78,212,587)	(59,494,595)	24,993,860	25,176,301	20,633,461	17,229,502	14,609,801	12,997,595	11,565,167	9,640,264	7,995,350	7,106,473	6,315,422	16,276,832
Cumul Discounted CF		(6,272,000)	(84,484,587)	(143,979,182)	(118,979,321)	(93,803,021)	(73,169,559)	(55,940,058)	(41,330,257)	(28,332,672)	(16,767,505)	(7,127,240)	868,110	7,974,583	14,290,005	30,566,838

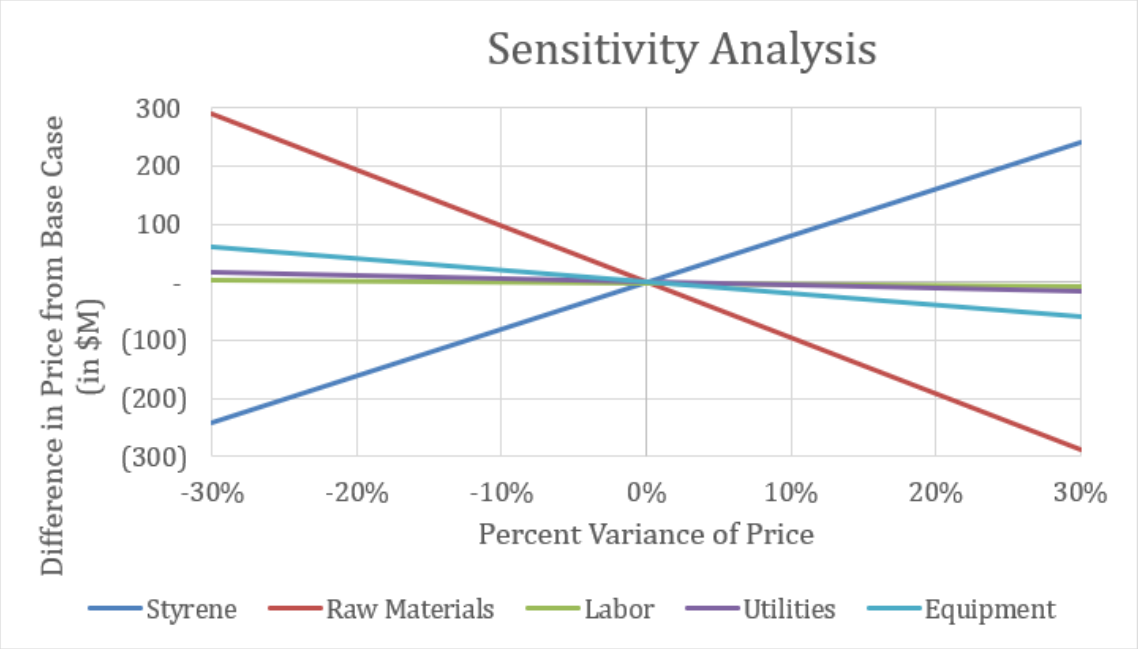
Summary Metrics					
NPV (12%)	30,566,838	AE (12%)	4,934,622.41	Conventional Payback Period	4.724216366
MARR	12%	DCFROR	16%	Discounted Payback Period	8.891423147

11. Thermodynamic Flowsheet



XVIII. Appendix B

1. Sensitivity Graph



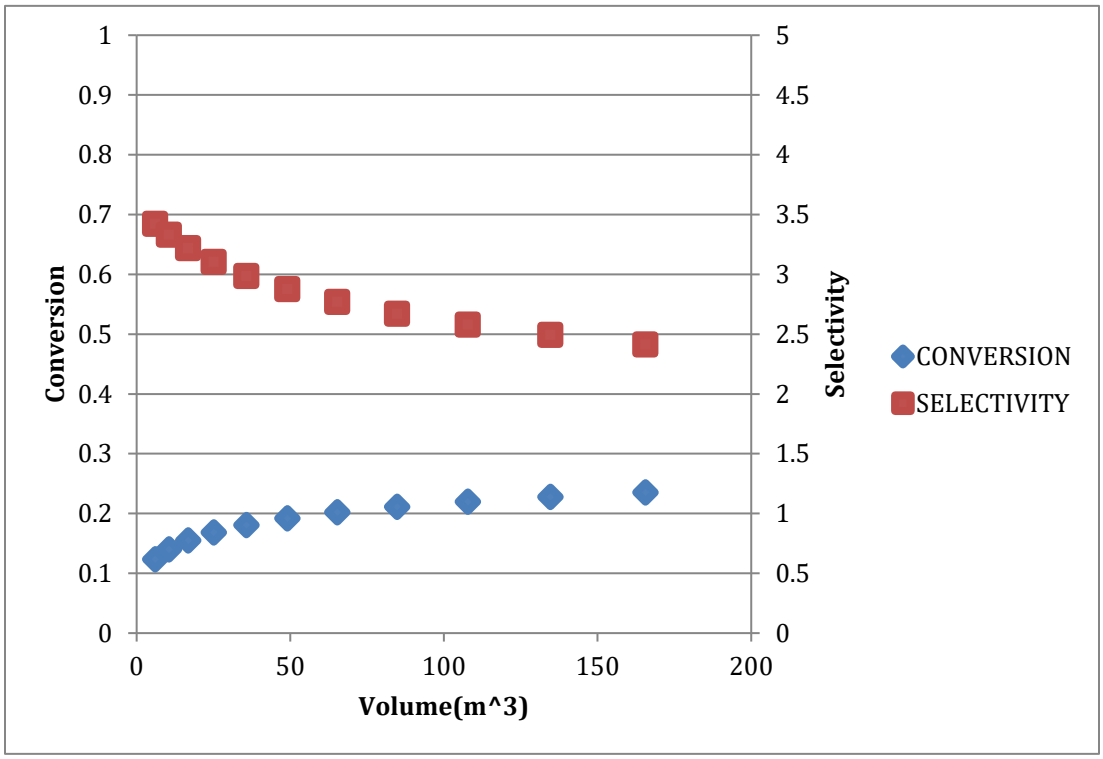
2. Economic Comparison (Reactor Type)

NPV Contribution	Isothermal	Adiabatic	Difference
Raw Materials	-$1178 M	-$1008 M	$170 M
Utilities	-$69 M	-$66 M	$3 M
FCI	-$137 M	-$190 M	-$53 M
NPV	-$320 M	-$264 M	$56 M

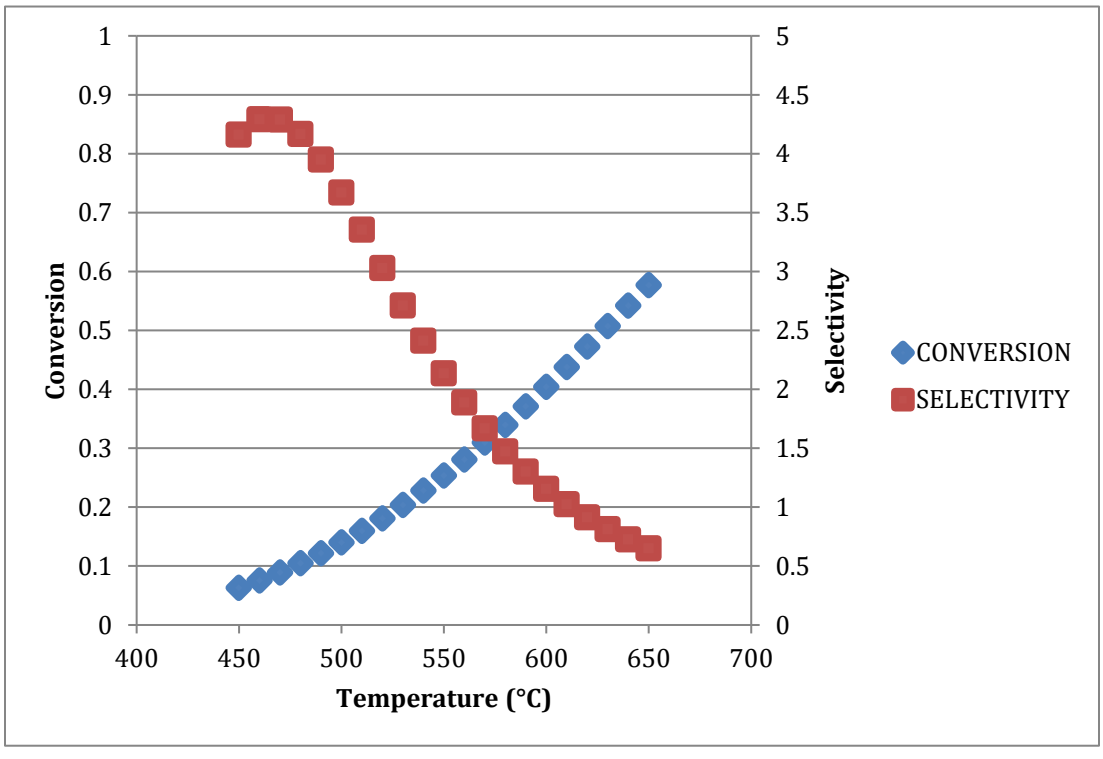
3. Economic Comparison (Reactor Conditions)

NPV Contribution	Adiabatic	Adiabatic with Changes	Difference
Raw Materials	-$1008 M	-$874 M	$134 M
Utilities	-$66 M	-$74 M	-$8 M
FCI	-$190 M	-$226 M	-$36 M
NPV	-$264 M	-$204 M	$60 M

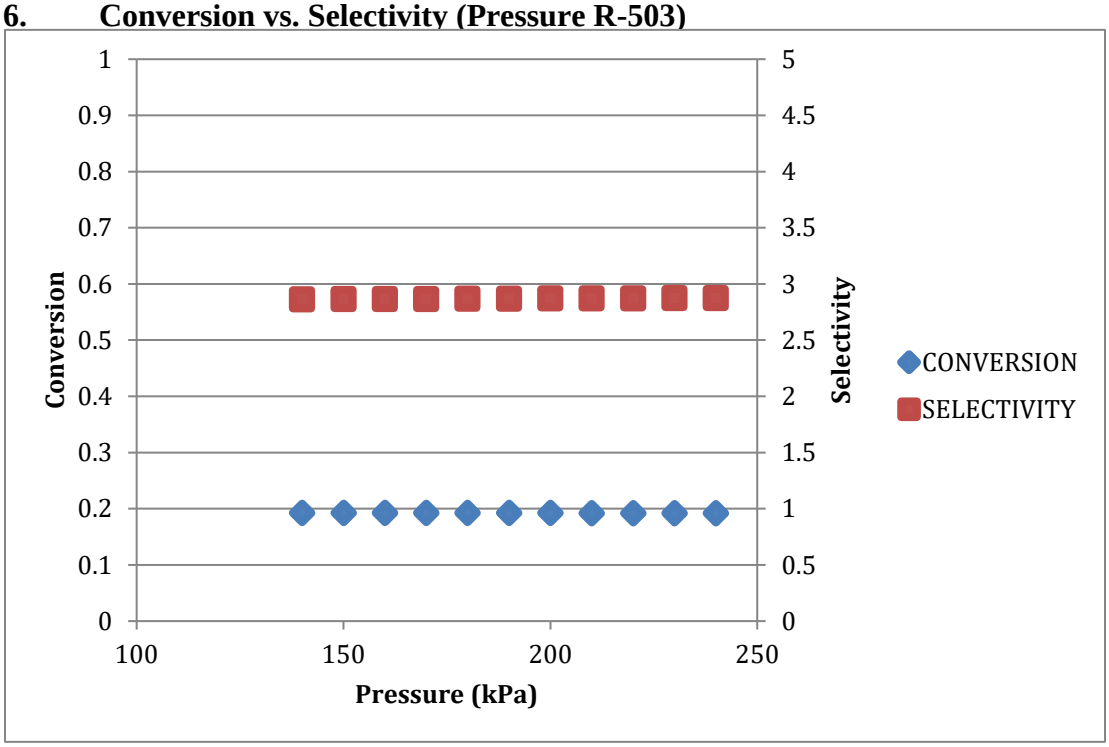
4. Conversion vs. Selectivity (Volume R-503)



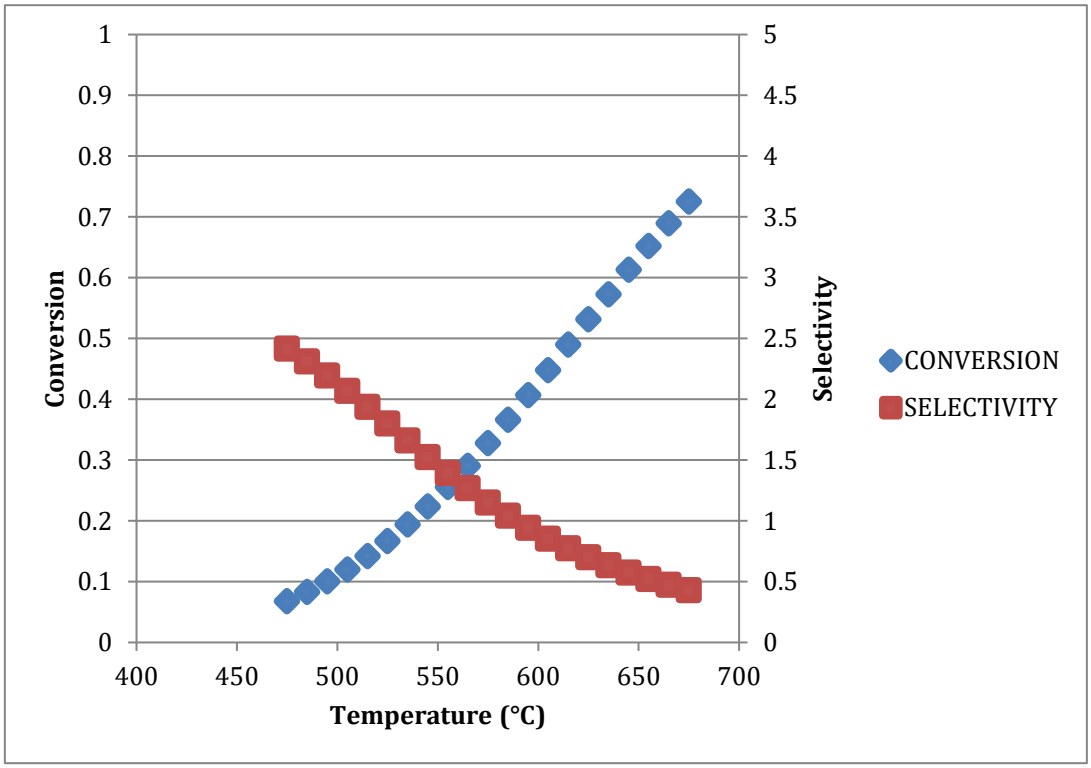
5. Conversion vs. Selectivity (Temperature R-503)



6. Conversion vs. Selectivity (Pressure R-503)



7. Conversion vs. Selectivity (Temperature R-503)



8. Economic Comparison (Materials of Construction)

NPV Contribution	No Material Change	With Material Changes	Difference
Raw Materials	-$875 M	-$875 M	-
Utilities	-$74 M	-$74 M	-
FCI	-$226 M	-$114 M	$112 M
NPV	-$204 M	-$39 M	$165 M

9. Economic Comparison (Heat Integration)

NPV Contribution	Without HI	With HI	Difference
Utilities	-$74 M	-$72 M	$2 M
FCI	-$114 M	-$114 M	$0.3 M
NPV	$16 M	$20 M	$4.1 M

10. Economic Comparison (Base Case vs. Optimized Case)

	Base Case	Optimized Case
NPV	-$320 M	$31 M
DCFROR	N/A	16%
AE	-$52 M	$5 M

XIX. Appendix C

1. Rate Laws

$$r_1 = 6.2 \exp\left(\frac{-90,981}{RT}\right) p_{eb}$$

$$r_2 = 6x10^{-5} \exp\left(\frac{-61,127}{RT}\right) p_{sty} p_{H_2}$$

$$r_3 = 2.71x10^{7} \exp\left(\frac{-207,989}{RT}\right) p_{eb}$$

$$r_4 = 6.45x10^{-4} \exp\left(\frac{-91,515}{RT}\right) p_{eb} p_{H_2}$$

Where p_i is the partial pressure of component *i* in Pa, T is the temperature in K, the activation energy is in J/mol, and the rate is in mole/(m^3 catalyst * second)

2. Notes About Fall Presentation Deficiencies

The engineering team addressed several deficiencies noted by the presentation panel in this report. First, we fixed errors in our PFDs which included changing the names of the adiabatic reactors to R-503 and R-504, aligning the input and output streams on the far left and far right sides of the page, and ensuring that stream 19 remained the fuel gas stream exiting the plant. The panel also noted that the temperature of the process is above the flash point of each component. This finished process safety section in the paper includes this. Lastly, the panel noted a lack of sources for why the team decided to use stainless

steel clad as the material for towers T-501 and T-502; therefore, after further research, the team selected carbon steel as the tower material and documented the source used in the works cited section.

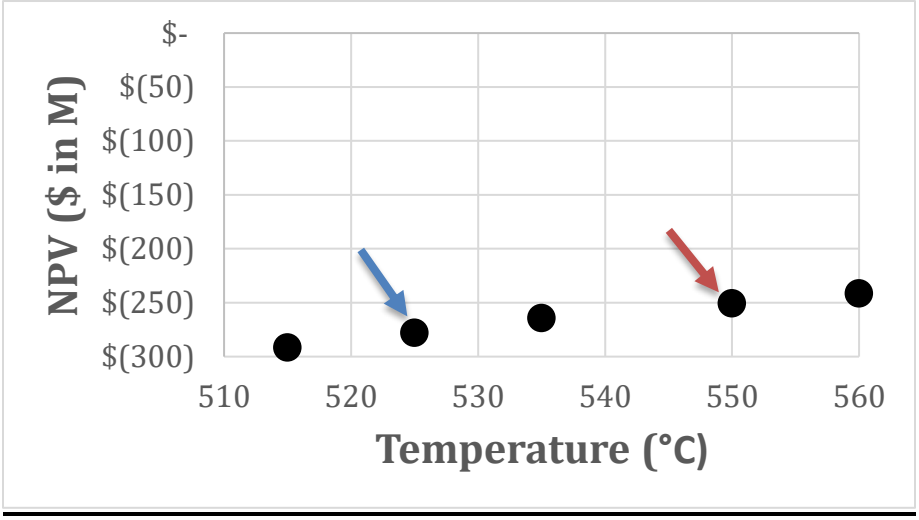
We also corrected calculation errors. For the presentation, the team made graphs showing the change in selectivity and conversion as temperature and pressure changed in the reactor section; however, we used the incorrect definition of selectivity. Originally, the engineering team defined it as the yield of styrene divided by the total amount of all side products (benzene and toluene) and by products (hydrogen, ethylene, and methane). Now, the definition is yield of styrene divided by only the side product total. In addition, a calculation issue in Excel occured when the team originally added tower T-503. The additional separation caused an increase in the raw materials cost for the total process when solving the mass balances, which did not make sense as it should only be separating the pre-existing stream. We corrected this by using a separate tab for the T-503 calculation.

Lastly, the most significant deficiency noted was that the team's graphs and tables were not effective. Our original tables put prices per year, one-time costs, and NPV in one place, and denoted the significance of the adjustment in the process with percent changes. We corrected all tables in Appendix B so they now display NPV contributions (the panel asked us to either put all the values in terms of NPV or estimated annual operating costs- EAOCs.) These figures are in the appendices to make them accessible to the reader but also to keep them separate so that they do not become a distraction. In addition, the graphs shown below

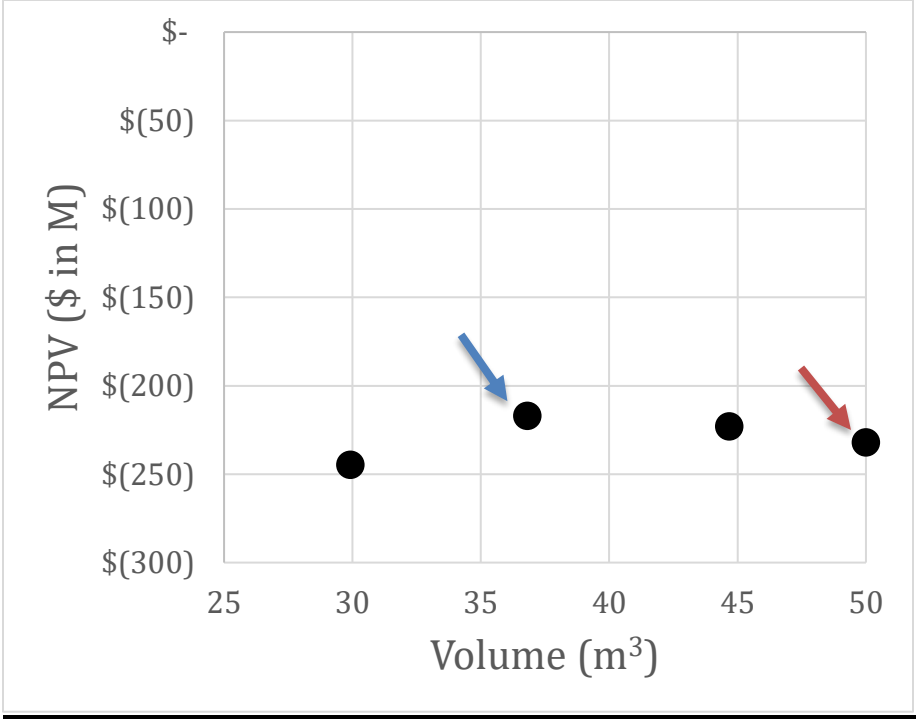
were made for the presentation; however, the NPV values are now incorrect as it is found that the team did not remove the utility cost for the isothermal reactors once they changed to adiabatic. However, despite this mistake, the trends observed in the graphs did not change and this still influenced the team's design choices. If given more time, the team would correct these to properly reflect the accurate NPV.

a. <u>R-503: Change in Temperature vs. NPV</u>

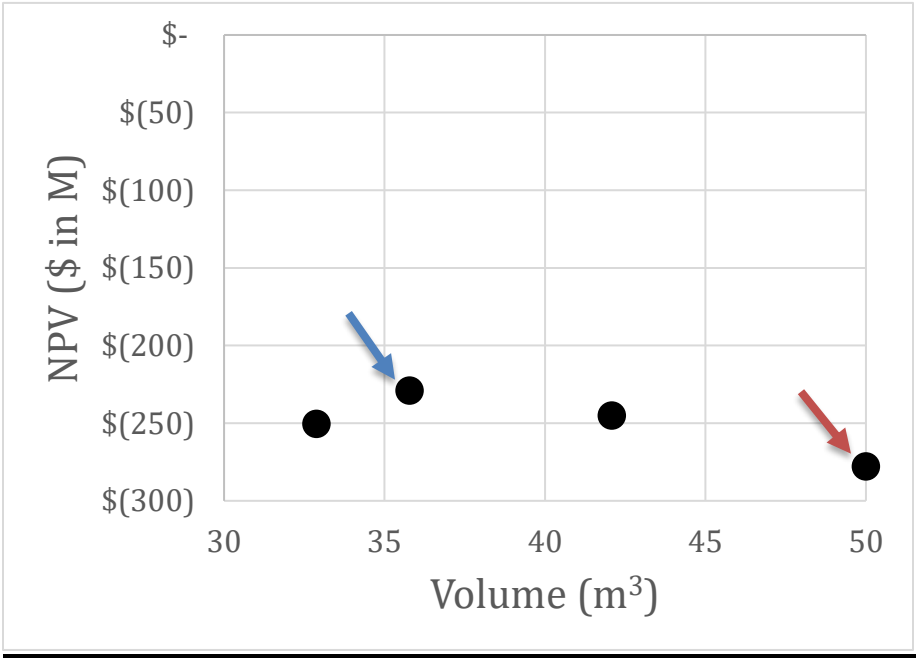
***Red indicates Base Case/Blue indicates Change**



b. <u>R-503: Change in Volume vs. NPV</u>



c. **R-504: Change in Volume vs. NPV**

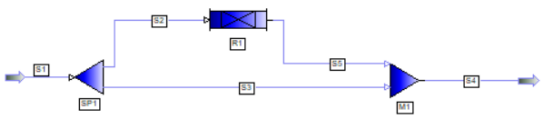


3. Reynolds Number and Archimedes Number Formulas

$$\mathrm{Re}_{p,mf} = \frac{u_{mf} d_p \rho_g}{\mu_g} = [1135.69 + 0.0408 Ar]^{0.5} - 33.7$$

where Ar is the Archimedes number, $Ar = \frac{d_p^3 (\rho_s - \rho_g) \rho_g g}{\mu_g^2}$; d_p, the particle diameter; ρ_g, the gas density; μ_g, the gas viscosity; ρ_s, the catalyst density; and g, the acceleration of gravity.

4. Fluidized Bed Reactor Pro/II Simulation



Stream Name		S4
Stream Description		
Phase		Vapor
Temperature	C	549.9880
Pressure	KPA	133.5096
Enthalpy	M*KJ/HR	294.8993
Molecular Weight		27.0229
Mole Fraction Vapor		1.0000
Mole Fraction Liquid		0.0000
Rate	KG-MOL/HR	4012.000
Fluid Rates	KG-MOL/HR	
EBENZENE		291.6935
H2O		3466.8000
STYRENE		90.7019
H2		65.1952
BENZENE		24.1978
TOLUENE		27.4067
ETHYLENE		21.6978
METHANE		24.3067

5. Works Cited

[1] Turton, Richard. Analysis, Synthesis, and Design of Chemical Processes. Upper Saddle River, N.J: Prentice Hall, 2003. Print.

[2] "Hydrogen Embrittlement." *NACE.org*, NACE, www.nace.org/Corrosion-Central/Corrosion-101/Hydrogen-Embrittlement/.

[3] Cocco, Ray & B. Reddy Karri, S & Knowlton, Ted. (2014). Introduction to Fluidization. Chemical Engineering Progress. 110. 21-29.